Quininic acid

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		**Training (75%)**		**Test (25%)**	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 183 °C

Global applicability domain: Inside

Local applicability domain index: 5.14e-01

Confidence level: 5.73e-01

Nearest Neighbors from the Training Set

Image not found
Indoprofen
Measured: 214
Predicted: 197

Image not found
Oxaprozin
Measured: 161
Predicted: 176

Image not found
Indobufen
Measured: 183
Predicted: 185

Image not found
Zomepirac
Measured: 179
Predicted: 158